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Liu, Fawang, Anh, Vo, Turner, Ian, & Zhuang, Pinghui (2004) Numerical simulation for solute transport in fractal porous media. *ANZIAM Journal*, *45*, C461-C473.

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Numerical simulation for solute transport in fractal porous media

F. Liu[†*] V. Anh[†] I. Turner[†] P. Zhuang[*]

March 30, 2004

Abstract

A modified Fokker-Planck equation (MFPE) with continuous source for solute transport in fractal porous media is considered. The dispersion term of the governing equation uses a fractional-order derivative and the diffusion coefficient can be time- and scale-dependent. In this paper, numerical solution of the MFPE is proposed. The effects of different fractional orders and fractional power functions of time and distance are numerically investigated. The results show that motions with a heavy-tailed marginal distribution can be modelled by equations that use fractional-order derivatives and/or time- and scale-dependent dispersivity.

Contents

[*]Department of Mathematics, Xiamen University, Xiamen 361005, CHINA. `mailto:fwliu@xmu.edu.cn`

[†]School of Mathematical Sciences, Queensland University of Technology, QlD. 4001, AUSTRALIA

1 Introduction

Solutes that move through fractal porous media commonly exhibit large deviations from the stochastic process of Brownian motion, hence do not generally follow a Fickian, second-order, governing equation. Recent theories devised to explain non-Fickian dispersion in turbulent and chaotic systems [18, 17] begin with the assumption that particle excursion distance and velocities are likely to have large, even infinite, variance. The transition probabilitry densities are then shown to converge relatively quickly to a non-Gaussian density.

The most common methods to incorporate relatively large particle motions include treating the parameters and dependent variables of the advection dispersion equation (ADE) as random and correlated, which leads to a time- and scale-dependent effective dispersion tensor [4, 5, 14, 19]. The literature highlights a great deal of effort expended to explain the scaling of parameters. Far less work has been done to examine the structure of the governing equation, especially the suitability of the differential equation itself. The Fokker-Planck equation (FPE) has been modified to use fractional derivatives and/or time- and scale-dependent dispersivity [1, 2, 19]. In this paper, a modified Fokker-Planck equation (MFPE) with continuous source is considered. The dispersion term of the governing equation uses a fractional-order derivative and/or time-, scale-dependent dispersivity. The MFPE is difficult to solve accurately using standard discretisation methods. In this paper, we concentrate on describing the numerical methods without studying the convergence and stablility of the methods from the theoretical point of view. In the numerical solution, the *Riemann-Liouville* and *Grünwald-Letnikov* definitions and a special finite difference scheme are used for the spatial approximation. The MFPE is transformed into a system of ordinary differential equations (ODE), which is then solved using the backward differentiation formulas of order one through five [3]. Numerical results for the cases of fractional derivative and spatially symmetric plumes, and FPE with time- and scale-dependence are derived for comparison with the similarity solution. In this study we examine and show that the MFPE, including the fractional-order derivative and time-, scale-dependent dispersivity, is also a useful model for transport with heavy-tailed motions.

2 Factional Fokker-Planck equations

The numerical solution of differential equations of integer order has for a long time been a standard topic in numerical and computational mathematics. However, in spite of a large number of recently formulated applied problems, the state is far less advanced for fractional-order differential equations.

Recently, the fractional Fokker-Planck equations (FFPE) have received a great deal of attention [1, 2]. These derivatives are nonlocal operators that incorporate spatial and/or temporal memory. In particular, a spatial fractional derivative describes particles that move with long-range spatial dependence or high velocity variability.

A special case of the FFPE may be written as [1, 2, 12]:

$$\frac{\partial C}{\partial t} = -\nu \frac{\partial C}{\partial x} + \left(\frac{1}{2} + \frac{\beta}{2}\right) D D^{\alpha}_{a+} C + \left(\frac{1}{2} - \frac{\beta}{2}\right) D D^{\alpha}_{b-} C, \tag{1}$$

where ν is the drift of the process, that is, the mean advective velocity, D is the coefficient of dispersion, $1 < \alpha < 2$ is the order of fractional differentiation, $-1 \leq \beta \leq 1$ indicates the relative weight of forward versus backward transition probability. Here $D^{\alpha}_{a+} f(x)$ and $D^{\alpha}_{b-} f(x)$ are left-handed and right-handed *Riemann-Liouville* fractional derivatives [16] of order α, $0 \leq n - 1 < \alpha < n$, n being an integer:

$$D^{\alpha}_{a+} f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x \frac{f(\xi) d\xi}{(x-\xi)^{\alpha-n+1}},$$

$$D^{\alpha}_{b-} f(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_x^b \frac{f(\xi) d\xi}{(\xi-x)^{\alpha-n+1}}.$$

In this section, we consider the FFPE (1) with a continuous source.

It is a very difficult task to solve fractional partial differential equations. Some numerical techniques have been proposed to approximate the fractional derivative (Podlubny [16]); Oldham and Spanier [15] discussed some techniques for handling differintegration of noninteger order.

In this section we consider the case of constant coefficient of dispersion. We use the algorithms for affecting differintegration for the evaluation of fractional-order derivatives. This approach has been adopted previously for a wide class of real physical and engineering applications. We use two definitions of fractional derivative: *Riemann-Liouville* and *Grünwald-Letnikov* [13, 15, 16]. There exists a link between the *Riemann-Liouville* and *Grünwald-Letnikov* approaches to differentiation of arbitrary real order.

Using the *Grünwald-Letnikov* definition [15], we have

$$D_{a+}^{\alpha} f(x) = \sum_{j=0}^{n-1} \frac{f^{(j)}(a)(x-a)^{j-\alpha}}{\Gamma(1+j-\alpha)} + \frac{1}{\Gamma(n-\alpha)} \int_a^x \frac{f^{(n)}(\xi)d\xi}{(x-\xi)^{\alpha-n+1}} \tag{2}$$

and similarly for $D_{b-}^{\alpha} f(x)$.

The relationship between the *Riemann-Liouville* and *Grünwald-Letnikov* definitions also has another consequence that is very important for the numerical approximation of fractional-order differential equations, formulation of applied problems, manipulation with fractional derivatives and the formulation of physical meaningful initial-value and boundary-value problems for fractional-order differential equations. This relationship allows the use of the *Riemann-Liouville* definition during problem formulation, and then turn to the *Grünwald-Letnikov* definition for obtaining the numerical solution.

The spatial approximation can be derived as follows:

Let $h = (b-a)/L$, $x = x_l = a + lh$, $f_0 = f(x - lh) = f(a)$, $f_1 = f(x-(l-1)h) = f(a+h)$, ... , $f_{l-j} = f(x - jh)$, ... , $f_l = f(x) = f(a+lh)$, ... , $f_{l+j} = f(x+jh)$, ... , $f_{L-1} = f(b-h)$, ... , $f_L = f(b)$.

Then, using the *Grünwald-Letnikov* derivative definition and Oldham and Spanier's technique [15], we obtain the following scheme (GLS) for $1 < \alpha < 2$, $(l = 1, ..., L-1)$:

$$\begin{aligned} \frac{dC_l}{dt} &= -\mu \frac{(C_l - C_{l-1})}{h} + \left(\frac{1}{2} + \frac{\beta}{2}\right) \frac{Dh^{-\alpha}}{\Gamma(3-\alpha)} \left\{ \frac{(1-\alpha)(2-\alpha)C_0}{l^{\alpha}} + \frac{(2-\alpha)}{l^{\alpha-1}}(C_1 - C_0) \right. \\ &\quad \left. + \sum_{j=0}^{l-1} (C_{l-j+1} - 2C_{l-j} + C_{l-j-1})[(j+1)^{2-\alpha} - j^{2-\alpha}] \right\} \\ &\quad + \left(\frac{1}{2} - \frac{\beta}{2}\right) \frac{Dh^{-\alpha}}{\Gamma(3-\alpha)} \left\{ \frac{(1-\alpha)(2-\alpha)C_L}{(L-l)^{\alpha}} + \frac{(2-\alpha)}{(L-l)^{\alpha-1}}(C_L - C_{L-1}) \right. \\ &\quad \left. + \sum_{j=0}^{L-l-1} (C_{l+j-1} - 2C_{l+j} + C_{l+j+1})[(j+1)^{2-\alpha} - j^{2-\alpha}] \right\}. \end{aligned} \tag{3}$$

3 FPE with time- and scale-dependent dispersivity

In this section, we consider the time- and scale-dependent FPE (TSFPE)

$$\frac{\partial C}{\partial t} = -\nu \frac{\partial C}{\partial x} + \frac{\partial}{\partial x}\left[D(x,t)\frac{\partial C}{\partial x}\right], \tag{4}$$

where $D(x,t)$ is the dispersion coefficient that is assumed to have the following form:

$$D(x,t) = D_1 t^{\lambda} x^m, \lambda > -1, m \geq 0, \tag{5}$$

and D_1 is a constant.

The similarity solution of the TSFPE with continuous source and $m = 1 - \lambda$ has been obtained previously [19]:

$$C(x,t) = \frac{c_0 \int\limits_{x/t}^{\infty} \xi^{-m} exp\left[\frac{\nu \xi^{1-m}}{(1-m)D_1} - \frac{\xi^{2-m}}{(2-m)D_1}\right] d\xi}{\int\limits_{0}^{\infty} \xi^{-m} exp\left[\frac{\nu \xi^{1-m}}{(1-m)D_1} - \frac{\xi^{2-m}}{(2-m)D_1}\right] d\xi}, \quad m \neq 1, 2. \tag{6}$$

The special finite difference approximation and upwind scheme (SFDAUS) can be applied directly to the TSFPE (4) to obtain the following system of ordinary differential equations:

$$\frac{dC_l}{dt} = -\nu \frac{C_l - C_{l-1}}{h} + \frac{D_{l+\frac{1}{2}} \frac{C_{l+1} - C_l}{h} - D_{l-\frac{1}{2}} \frac{C_l - C_{l-1}}{h}}{h}, \tag{7}$$

where $D_{l\pm\frac{1}{2}} = \frac{1}{2}\left[D(x_{l\pm 1}, t) + D(x_l, t)\right]$.

4 Numerical techniques

The method of lines (MOL) is a well-known technique for solving parabolic-type partial differential equations. Brenan *et al.* [3] developed the differential/algebraic system solver (DASSL), which is based on the backward difference formulas (BDF). DASSL approximates the derivatives using the kth order BDF, where k ranges from one to five. The stepsize h and order k are chosen based on the behaviour of the solution.

In this work, we used DASSL as our ODE solver. This technique has been used to solve a variety of important problems in the past, including the solutions of adsorption problems involving steep gradients in bidisperse particle [6], hyperbolic models of transport in bidisperse solids [7], transport problems involving steep concentration gradients[8], and modelling saltwater intrusion into coastal aquifers [9, 10].

5 Results and discussion

In this section, several examples for the MFPE are presented, which demonstrate the flexibility of the above methods. These numerical methods have

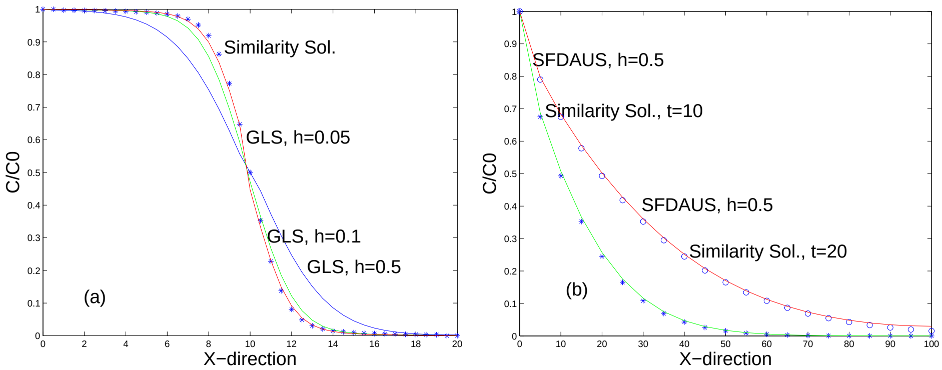

Figure 1: Comparison of similarity solution and numerical solution (a) using GLS for FFPE with $\alpha = 1.7, \beta = 0$, showing the effect of h (b) using SFDAUS for TSFPE with $\lambda = 0.5, m = 0.5$

been implemented in Fortran 77. The following initial and boundary conditions are used throughout this section:

$$t = 0, \ \ C = 0; x = a = 0, \ \ C = C_0; x = b \to \infty, \ \ \frac{\partial C}{\partial x} = 0. \tag{8}$$

5.1 FFPE $(1 < \alpha < 2, \beta = 0)$ using GLS

We consider the FFPE (1) with the continuous source (8).

Using the symmetric property, the similarity solution for the FFPE with $\beta = 0$ was obtained by Benson *et al.* [2]:

$$\frac{C}{C_0} = \frac{1}{2}\left[1 - serf_a\left\{\frac{x - \nu t}{\sqrt{|\cos(\pi\alpha/2)|Dt}}\right\}\right], \tag{9}$$

where we define the α-stable error function, $serf_a$, similarly to the error function, that is, twice the integral of a symmetric α-stable density from 0 to the argument z :

$$serf_a(z) = 2\int_0^z f_a(\xi)d\xi, \tag{10}$$

$f_\alpha(\xi)$ being the standard, symmetric, α -stable density.

In Figure 1(a), the similarity solution (9) and the numerical solutions using the GLS for $\alpha = 1.7$, $\beta = 0$, $D = 0.1$, $\nu = 1.0$, $b = X = 20$, $t = 10$ are shown, respectively. Figure 1(a) also shows the effect of spatial step length h . From Figure 1(a), it can be seen that the GLS is convergent. The numerical solution of the GLS is in good agreement with the similarity solution.

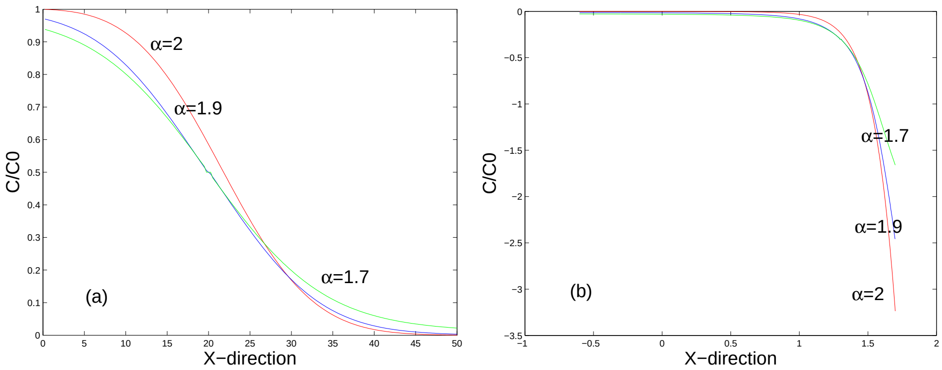

Figure 2: Numerical solution of FFPE using GLS with $v = 1, D = 2, t = 20$, showing the effect of α and heavy-tailed character: (a) linear axes; (b) log-log axes.

5.2 FPE with time- and scale-dependent dispersivity

We consider the TSFPE (4) with the continuous source (8).

In Figure 1(b), the similarity solution (6) and the numerical solutions (using SFDAUS with $h = 0.5$) for $t = 10$ and $t = 20$ are shown, respectively. In Figure 1(b), all curves use $\alpha = 2$, $D_1 = 2.0$, $\nu = 1.0$, $m = 0.5$, $\lambda = 0.5$, $X = 100$. From Figure 1(b), it can be seen that the numerical solution (SFDAUS) of the TSFPE is again in good agreement with the similarity solution.

5.3 Properties of MFPE

We next examine the properties of MFPE. Figure 2 shows standard $\alpha-$stable distribution functions for $\alpha = 1.7$, 1.9 and 2, and the effect of the fractional-order derivative α for $D = 2.0$, $\nu = 1.0$, $t = 20$ in the linear axes and $\log - \log$ axes, respectively. From Figure 2 it can be seen that FFPE with α-stable densities has heavier tails in comparison to the traditional second-order FPE. As the value of α descreases from a maximum of 2, the probability density displays longer and longer tails.

Figure 3 shows the effect of λ and m for $D_1 = 2.0$, $\nu = 2.0$, $t = 20$ in the linear axes and $\log - \log$ axes, respectively. From Figure 3 , it can be seen that when $D(x, t)$ is a dispersion coefficient as a function of x and t, the concentration has a heavy-tailed behaviour.

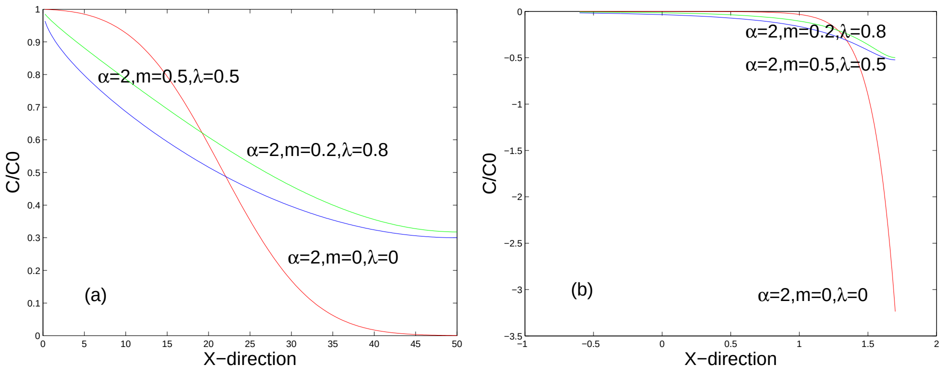

Figure 3: Numerical solution of TSFPE using SFDAUS with $\alpha = 2, v = 1, D = 2, t = 20$, showing the effect of λ and m, and heavy-tailed character: (a) linear axes; (b) log-log axes.

6 Conclusions

In this paper, numerical solutions of the modified Fokker-Planck equation with fractional derivative and time- and scale-dependent dispersivity have been developed. The effects of fractional order, time- and scale-dependent dispersivity have been numerically investigated. The correspondence between these heavy-tailed motions and transport equations that use fractional-order derivatives or time-, scale-dependent dispersivity has been described and demonstrated.

Acknowledgements: This research has been supported by the ARC SPIRT grant C10024101 and the National Natural Science Foundation of China grant 10271098.

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